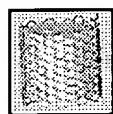
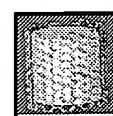


# Nanotube Research in David Tománek's Group

Research on carbon nanotubes in my group focusses on modeling the self-assembly and electronic properties of these systems. Recent advances in the synthesis of identical carbon nanotubes with a diameter of 1.4 nm, yet hundreds of microns in length, bear high promise for the application of these advanced materials in next-generation electronic nano-devices. Advanced computational techniques, including large-scale parallelizable molecular dynamics simulations of the growth mechanism and first-principles calculations of the electronic structure, are being applied to model the self-assembly and the electronic properties of these structures. Results will elucidate ways to direct and optimize growth conditions, mechanical and thermal stability, and the usefulness of nanotubes as perfect nanoscale conductors.



[... simulations of carbon nanotubes](#)



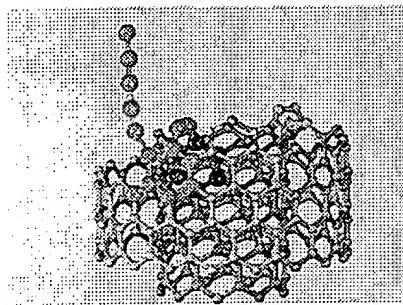
[... general information and press release of  
David Tomanek's invited talk at the 1997 APS March Meeting](#)

## Nanotube Publications - David Tománek's Group

1. G. Overney, W. Zhong, and D. Tománek, Structural Rigidity and Low Frequency Vibrational Modes of Long Carbon Tubules, *Z. Phys. D* **27**, 93-96 (1993).
2. D. Tománek, W. Zhong, and E. Krastev, Stability of Multi-Shell Fullerenes, *Phys. Rev. B* **48**, 15461 (1993).
3. Ting Guo, Pavel Nikolaev, Andrew G. Rinzler, David Tománek, Daniel T. Colbert, and Richard E. Smalley, Self-Assembly of Tubular Fullerenes, *J. Phys. Chem.* **99**, 10694 (1995).
4. A.G. Rinzler, J.H. Hafner, P. Nikolaev, L. Lou, S.G. Kim, D. Tománek, P. Nordlander, D.T. Colbert, and R.E. Smalley, Unraveling Nanotubes: Field Emission from an Atomic Wire, *Science* **269**, 1550 (1995).
5. David Tománek, The growth and the death of carbon fullerenes and nanotubes. In "*Large Clusters of Atoms and Molecules*", ed. by T. P. Martin, Nato ASI series vol. 313 (Kluwer Academic Publishers, Netherlands, 1996), p. 405.
6. Andreas Thess, Roland Lee, Pavel Nikolaev, Hongjie Dai, Pierre Petit, Jerome Robert, Chunhui Xu, Young Hee Lee, Seong Gon Kim, Daniel T. Colbert, Gustavo Scuseria, David Tománek, John E. Fischer, and Richard E. Smalley, Crystalline ropes of metallic carbon nanotubes, *Science* **273**, 483 (1996).
7. Seong Gon Kim, Young Hee Lee, Peter Nordlander, and David Tománek, Disintegration of finite carbon chains in electric fields, *Chemical Physics Letters* **264**, 345-350 (1997).
8. Young Hee Lee, Seong Gon Kim, and David Tománek, Field-induced unraveling of carbon nanotubes, *Chem. Phys. Lett.* **265**, 667 (1997).
9. Young Hee Lee, Seong Gon Kim, and David Tománek, Catalytic growth of single-wall nanotubes: An *ab initio* study, *Phys. Rev. Lett.* **78**, 2393 (1997).
10. Young-Kyun Kwon, Young Hee Lee, Seong-Gon Kim, Philippe Jund, David Tománek, and Richard E. Smalley, Morphology and stability of growing multi-wall carbon nanotubes, *Phys. Rev. Lett.* **79**, 2065 (1997).
11. D. Östling, D. Tománek, and A. Rosén, Electronic structure of single-wall, multi-wall, and filled carbon nanotubes, *Phys. Rev. B* **55**, 13980-13988 (1997).
12. A. Rosén, D. Östling, P. Apell, and D. Tománek, From Astrophysics to Mesoscopic Physics - A Sightseeing

Tour in the World of Clusters and Fullerenes, in "Fullerenes and Photonics III", SPIE Proceedings volume 2854, edited by Zakya H. Kafafi, Proceedings of the Symposium of SPIE - The International Society for Optical Engineering - in Denver, CO, 5-6 August 1996, p. 2-16.

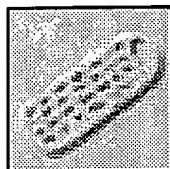
13. Young-Kyun Kwon, David Tománek, Young Hee Lee, Kee Hag Lee, and Susumu Saito, Do carbon nanotubes spin when bundled? *J. Mater. Res.* **13**, 2363-2367 (1998).
14. L.G. Bulusheva, A.V. Okotrub, D.A. Romanov, and D. Tománek, Electronic structure of (n,0) zigzag carbon nanotubes: Cluster and crystal approach, *J. Phys. Chem. A* **102**, 975-981 (1998).
15. Alexander V. Okotrub, Lyubov G. Bulusheva and David Tománek, X-ray spectroscopic and quantum-chemical study of carbon tubes produced by arc-discharge, *Chem. Phys. Lett.* **289**, 341-349 (1998).
16. Young-Kyun Kwon, Susumu Saito, and David Tománek, Effect of inter-tube coupling on the electronic structure of carbon nanotube ropes, *Phys. Rev. B* **58**, R13314 (1998).
17. David Tománek, Self-assembly and electronic structure of bundled single- and multi-wall nanotubes. In "*Electronic Properties of Novel Materials - Progress in Molecular Nanostructures*", Proceedings of the XII International Winterschool in Kirchberg, Tyrol, March 1998, edited by Hans Kuzmany, Jörg Fink, Michael Mehring, and Siegmar Roth, AIP Proceedings Vol. 442, pp. 159-163.
18. Young-Kyun Kwon, David Tománek, and Sumio Iijima, "Bucky-Shuttle" Memory Device: Synthetic Approach and Molecular Dynamics Simulations, *Phys. Rev. Lett.* **82**, 1470 (1999).
19. L.G. Bulusheva, A.V. Okotrub, D.A. Romanov, and D. Tománek, Electronic structure of carbon nanotubes, *Phys. Low-Dim. Struct. 3/4*, 107-133 (1998).
20. Young-Kyun Kwon and David Tománek, Electronic and Structural Properties of Multi-Wall Carbon Nanotubes, *Phys. Rev. B* **58**, R16001 (1998).
21. Petr Král and David Tománek, Laser driven atomic pump, *Phys. Rev. Lett.* **82**, 5373 (1999).
22. David Tománek, Self-assembly of carbon nanotubes, *Mol. Mat.* **10**, 9-16 (1998).
23. David Tománek, Interplay Between Structural and Electronic Properties of Carbon Nanotubes. In "*Collective Excitations in Fermi and Bose Systems*", Proceedings of the International Workshop on Collective Excitations in Fermi and Bose Systems in Serra Negra, São Paulo, Brazil, September 1998.
24. Mark Brehob, Richard Enbody, Young-Kyun Kwon, and David Tománek, The Potential of Carbon-Based Memory Systems. Proceedings of IEEE conference MTDT'99, 1999.
25. Stefano Sanvito, Young-Kyun Kwon, David Tománek, and Colin J. Lambert, Fractional quantum conductance in carbon nanotubes, *Phys. Rev. Lett.* **84**, 1974 (2000).
26. S. Sanvito, Y.-K. Kwon, D. Tománek, and C.J. Lambert, Quantum transport in inhomogeneous multi-wall nanotubes, Proceedings of the Nanotube-99 Conference in East Lansing, Michigan, July 24-27, 1999, (Kluwer, New York, 2000), pp. 333-348.
27. Young-Kyun Kwon and David Tománek, Orientational melting in carbon nanotube ropes, *Phys. Rev. Lett.* **84**, 1483 (2000).
28. Eugene J. Mele, Petr Král, and David Tománek, Coherent control of photocurrents in graphene and carbon nanotubes, *Phys. Rev. B* **61**, 7669 (2000).
29. V.V. Belavin, L.G. Bulusheva, A.V. Okotrub, and D. Tománek, Stability, electronic structure and reactivity of the polymerized fullerite forms (submitted for publication).
30. Savas Berber, Young-Kyun Kwon, and David Tománek, Unusually High Thermal Conductivity of Carbon Nanotubes, *Phys. Rev. Lett.* **84**, 4613 (2000).
31. Savas Berber, Young-Kyun Kwon, and David Tománek, Electronic and Structural Properties of Carbon Nano-Horns, *Phys. Rev. B* **62** (2000).
32. David Tománek, Electrical and Thermal Transport in Carbon Nanotubes. In "*Electronic Properties of Novel Materials - Molecular Nanostructures*", Proceedings of the XIV International Winterschool in Kirchberg, Tyrol, March 2000, edited by Hans Kuzmany, Jörg Fink, Michael Mehring, and Siegmar Roth.
33. Petr Král, E. J. Mele, and David Tománek, Photogalvanic Effects in Heteropolar Nanotubes, *Phys. Rev. Lett.* **85** (2000).



---

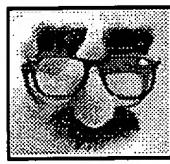
**David Tománek: Complete list of publications**

---



[... back to The Nanotube Site](#)

---



[... back to David Tomanek's home page](#)

---

Document <http://www.pa.msu.edu/~tomanek/nanotubes.html>

maintained by David Tomanek -  [tomanek@pa.msu.edu](mailto:tomanek@pa.msu.edu).